

Groundwater Transport Modeling Using Response Surface Modeling: Proof of Principle

Arthur S. Rood
June 2005

**Idaho
Cleanup
Project**

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Idaho Falls, Idaho 83415

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ABSTRACT

Numeric models of groundwater flow and transport can be time consuming and resource intensive to run even on modern computing systems. This is especially true if many contaminant sources and multiple contaminants are simulated. A method is proposed to reduce the computational requirements for simulation of multiple contaminants and multiple contaminant sources in an aquifer system. It uses the convolution integral coupled with source-receptor response functions and contaminant fluxes to the aquifer to estimate groundwater concentrations at selected receptor locations in the groundwater modeling domain. The entire process is termed response surface modeling. The approach retains most of the complexity of the flow and transport modeling performed using complex numerical models, although some simplifying assumptions are necessary. The model was demonstrated using a response function developed from a two-dimensional MODFLOW simulation of the Snake River Plain Aquifer.

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Groundwater Transport Modeling Using Response Surface Modeling: Proof of Principle

1. INTRODUCTION

Numeric models of groundwater flow and transport can be time consuming and resource intensive to run even on modern computing systems. This is especially true if many contaminant sources and multiple contaminants are simulated. A method is proposed to reduce the computational requirements for simulation of multiple contaminants and multiple contaminant sources in an aquifer system. This approach is based on the response function discussion in “A Review of Distributed Parameter Groundwater Management Modeling Methods” (Gorelick 1983). It uses the convolution integral coupled with source-receptor response functions and contaminant fluxes to the aquifer to estimate groundwater concentrations at selected receptor locations in the groundwater modeling domain. The entire process is termed response surface modeling. The approach retains most of the complexity of the flow and transport modeling performed using complex numerical models, although some simplifying assumptions are necessary.

2. METHODOLOGY

Consider the model domain illustrated in Figure 1. There are three sources within the domain and there are multiple contaminants within each source. Each source has a “footprint” where contaminants from the vadose zone enter the aquifer. There are eight receptor locations within the model domain. These locations can represent existing wells, future wells, and points of interest in the aquifer. For example, Receptor Numbers 1, 2, and 3 may not represent actual wells, but points in the aquifer where the maximum contaminant concentration in groundwater from an individual source is achieved.

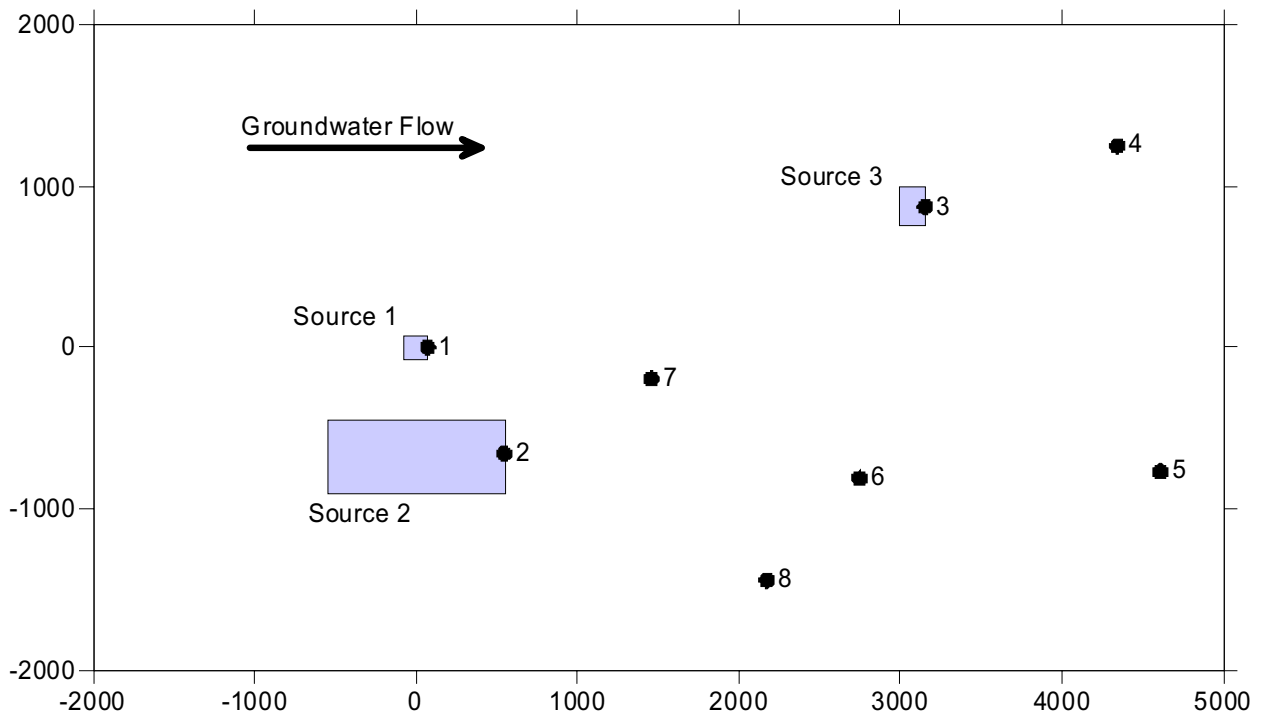


Figure 1. Hypothetical aquifer domain for demonstration of response surface modeling. The problem has three contaminant sources and eight receptor locations.

The breakthrough curve at each receptor to a unit mass input from each source is the response function. Response functions at the eight receptor locations for each of the three sources are shown in Figure 2. Note that for Source 3, only three receptors are shown, because the remaining receptors lie upgradient from Source 3 and are therefore unaffected by releases from the source. In this case, the response function is zero for all time. The response function is determined using a groundwater flow and transport model and represents the concentration in the aquifer as a function of time for a conservative, non-decaying, non-sorbing tracer of unit mass that is instantaneously released to the aquifer over the source footprint at the start of the simulation.

The contaminant loading rates to the aquifer can be arbitrary. An example of such loading rates is illustrated in Figure 3 for the three sources. These graphs represent the contaminant flux to the aquifer as a function of time for a single contaminant. However, multiple contaminants with varying sorption coefficients and decay products also can be simulated by developing source-loading rates for each contaminant.

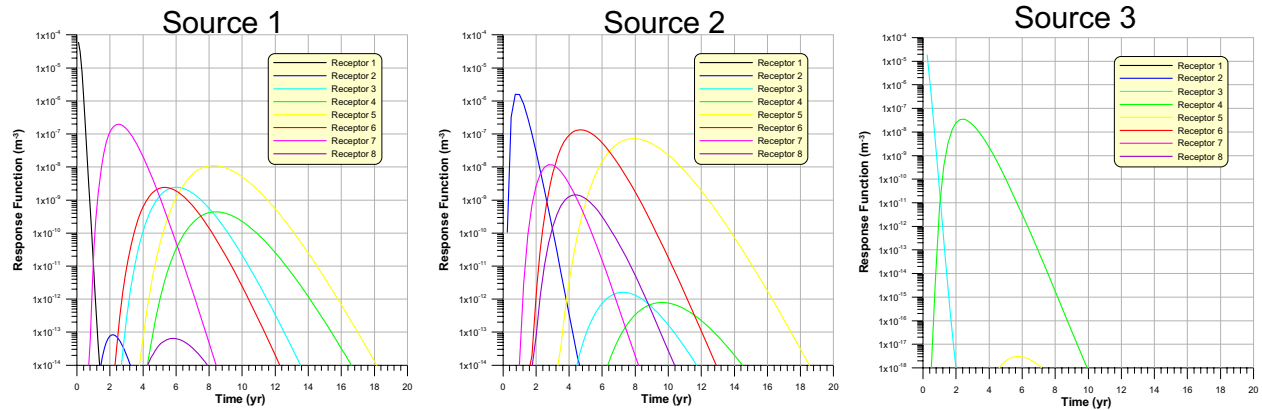


Figure 2. Response function for each receptor-source pair.

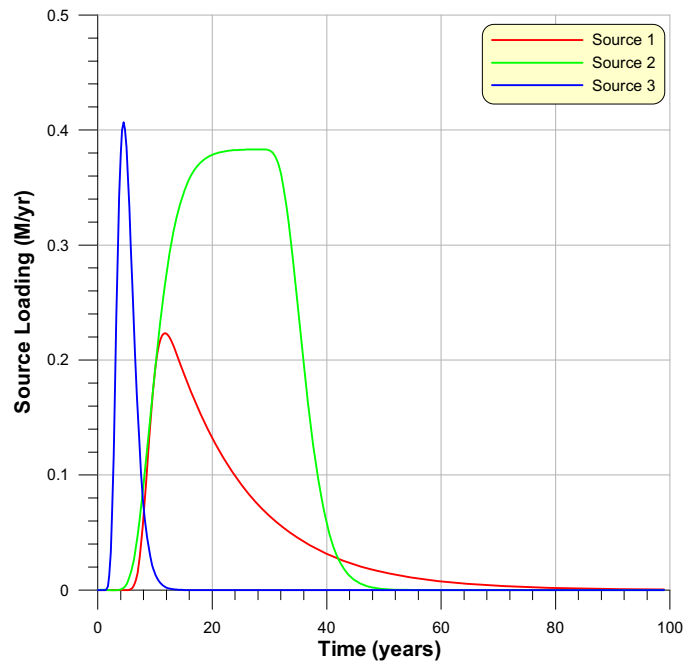


Figure 3. Example of source loading rates for each of the three sources.

The contaminant concentration in the aquifer at a given receptor location then represents the convolution of the source loading rates and the response function. That is, concentration in the aquifer can be represented by a series of individual “pulses” where the magnitude of the pulse is equal to the product of the source-loading rate at a given time, the response function at some time thereafter, and a time step. When summed together, the individual pulses form a continuous function of concentration over the time period of interest. The contaminant concentration (Equation [1]) is given by:

$$C_{i,j}(t) = \int_0^t RF_{i,j}(t-\tau) S_i(\tau) d\tau \quad (1)$$

where

$C_{i,j}(t)$ = aquifer concentration of a contaminant at time t for source i and receptor j ($M L^{-3}$)

$RF_{i,j}(t-\tau)$ = response function for source i and receptor j at time $t - \tau$ (L^{-3})

$S_i(\tau)$ = source-loading rate for source i at time τ ($M T^{-1}$)

i = source index

j = receptor index.

Equation (1) is valid for a non-decaying, non-sorbing contaminant. The quantity $t - \tau$ is the “age” of the pulse. To account for the decay and sorptive properties of different contaminants, several simplifying assumptions are made:

- Sorption is uniform throughout the aquifer
- Decay is constant throughout the aquifer
- Parent and progeny travel at the same rate in the aquifer.

The aquifer concentration for a decaying and sorbing contaminant that may generate decay products in transit (Equation [2]) is given by:

$$C_{i,j,k}(t) = \frac{1}{Rd_k} \int_0^t RF_{i,j} \left(\frac{t-\tau}{Rd_1} \right) S_{i,1}(\tau) DIF_k(t-\tau) d\tau \quad (2)$$

where

$C_{i,j,k}(t)$ = concentration of decay product k at time t for source i and receptor j ($M L^{-3}$)

$RF_{i,j}(t-\tau)$ = response function for source i and receptor j at time $t - \tau$ (L^{-3})

$S_{i,1}(\tau)$ = source-loading rate of parent ($k = 1$) for source i at time τ ($M T^{-1}$)

Rd_k = the retardation factor for product k , [$k=1$ for parent] (unitless)

DIF_k = decay-ingrowth factor for decay product k at time $t - \tau$ (unitless)

k = decay product index, [$k=1$ for parent].

The decay-ingrowth factor is the activity of decay product k present at time $t - \tau$ relative to the original parent activity released at time τ . The index k relates to the decay chain where $k = 1$ for the parent. For a single decay species with no progeny, the decay ingrowth factor is simply $\exp[-\lambda(t - \tau)]$. For a decay product other than the parent, the decay-ingrowth factor (Equation [3]) is given by:

$$DIF_k(t) = \frac{\lambda_k}{\lambda_1} \left[\left(\prod_{i=1}^{k-1} \lambda_i \right) \sum_{i=1}^k \frac{e^{-\lambda_i t}}{\prod_{\substack{j \neq i \\ j=1}}^i (\lambda_j - \lambda_i)} \right] \quad (3)$$

where

λ_1 = decay constant for the parent (T^{-1})

λ_k = decay constant for the k^{th} progeny (T^{-1})

t = age of pulse (T).

The total contaminant concentration from all sources is evaluated by superposition of each source-receptor pair. That is, the contaminant concentration at a given receptor location from multiple sources is the sum of the concentration from each individual source (Equation [4]).

$$C_{j,k}(t) = \sum_{i=1}^n C_{i,j,k}(t) \quad (4)$$

where

n is the number of sources considered in the model domain.

3. COMPUTER PROGRAM FOR CALCULATING THE CONVOLUTION INTEGRAL

Equations 1–4 were coded into a FORTRAN program that calculated concentration time histories for each source-receptor pair and then summed the concentration across all sources at each receptor. Inputs to the program include the source-loading rates, response functions, integration control variables, and output times. Source-loading rates and response functions are read into the program as tabular time-value entries. Integration is performed using a Simpson Rule algorithm described in *Numerical Recipes: The Art of Scientific Computing* (Press et al. 1996). Source-loading rates and response functions are linearly interpolated between data points to form a continuous function. Linear interpolation is performed using a routine described in Press et al. (1996).

4. SAMPLE APPLICATION

The model domain, sources areas, source-loading rates, and receptors that are illustrated in Figures 1–3 were used to demonstrate the methodology. Response functions were generated using the GWSCREEN code (Rood 1999). The GWSCREEN model combines a source release model, a one-dimensional unsaturated transport model, and a three-dimensional aquifer transport model assuming

unidirectional flow in a homogeneous and isotropic aquifer of infinite lateral extent and finite thickness. The source-loading rates illustrated in Figure 3 were used in the simulation and the contaminant was assumed to be non-decaying and non-sorbing (i.e., $\lambda \sim 1/\infty$, $Rd = 1$).

Figure 4 shows the concentration time histories at each of the receptors for each individual source and the total concentration from all sources. The graph for Source 1 (upper left graph of Figure 4) includes a plot of the concentrations determined using Equation 2 and the corresponding values calculated with GWSCREEN.

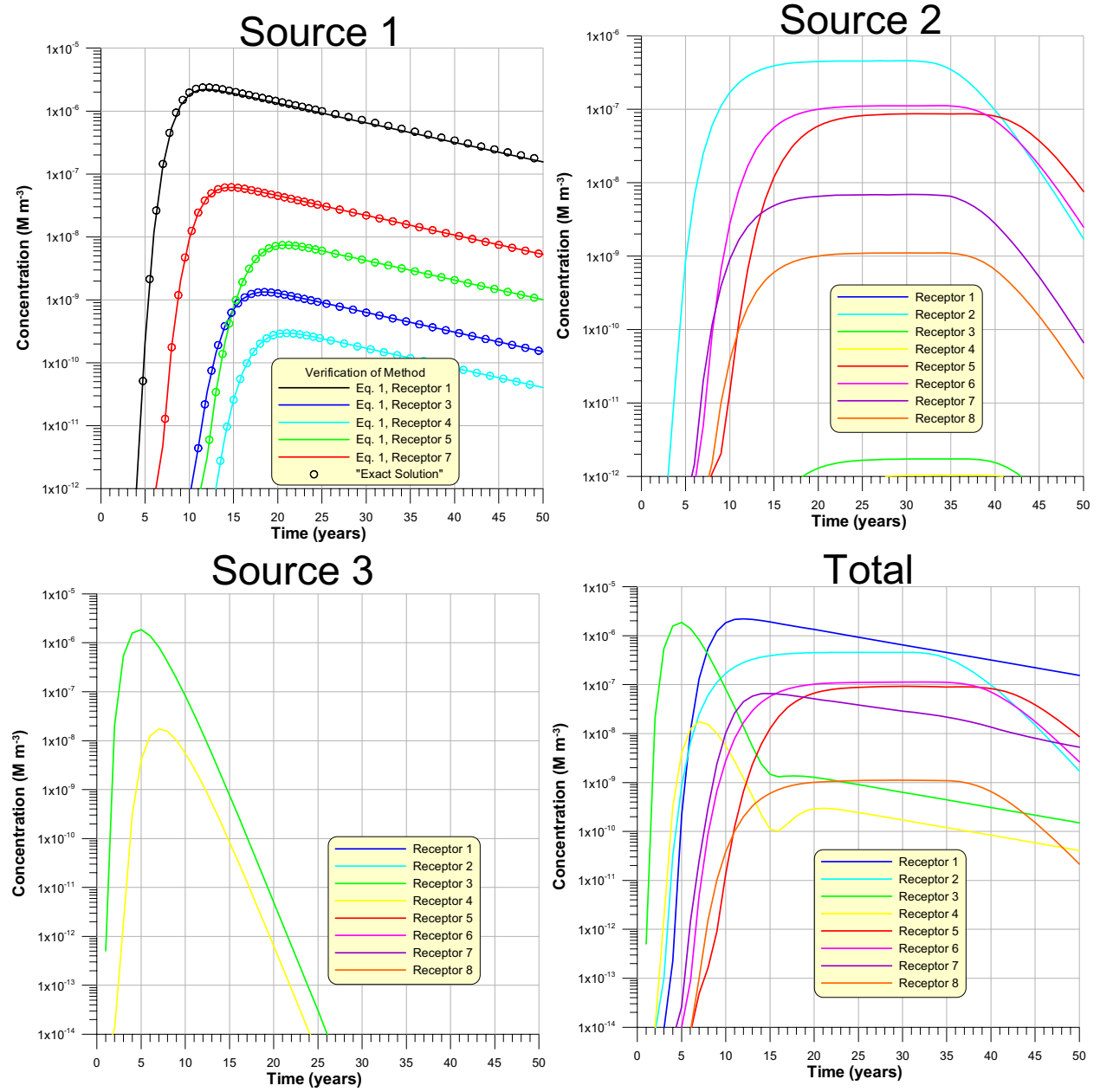


Figure 4. Contaminant concentration as a function of time at each receptor location for all individual sources and total as determined by Equation (4).

Figure 5 shows a comparison of concentrations as a function of time for Source 1 and a contaminant having a retardation factor of 2. This figure can be compared to the graph for Source 1 in Figure 4 that represents a contaminant with a retardation factor of 1. The source-loading rates were the same for both simulations, but a retardation factor of 2 in the aquifer was used in Figure 5. The solution using GWSCREEN also is shown for comparison. Qualitatively, there is very little difference between the “exact” solution determined with GWSCREEN and the response function approach discussed herein.

5. APPLICATION TO THE SNAKE RIVER PLAIN AQUIFER

The response surface model previously described and demonstrated with GWSCREEN was applied to the Waste Area Group 10 (WAG) 10 groundwater model. The WAG 10 groundwater model consists of the United States Geological Survey groundwater flow code and MODFLOW coupled with the MT3D transport code. Both codes are incorporated in the Groundwater Modeling System graphical user interface. Simulations were based on a two-dimensional aquifer flow and transport simulation. Aquifer depths were variable across the modeling domain.

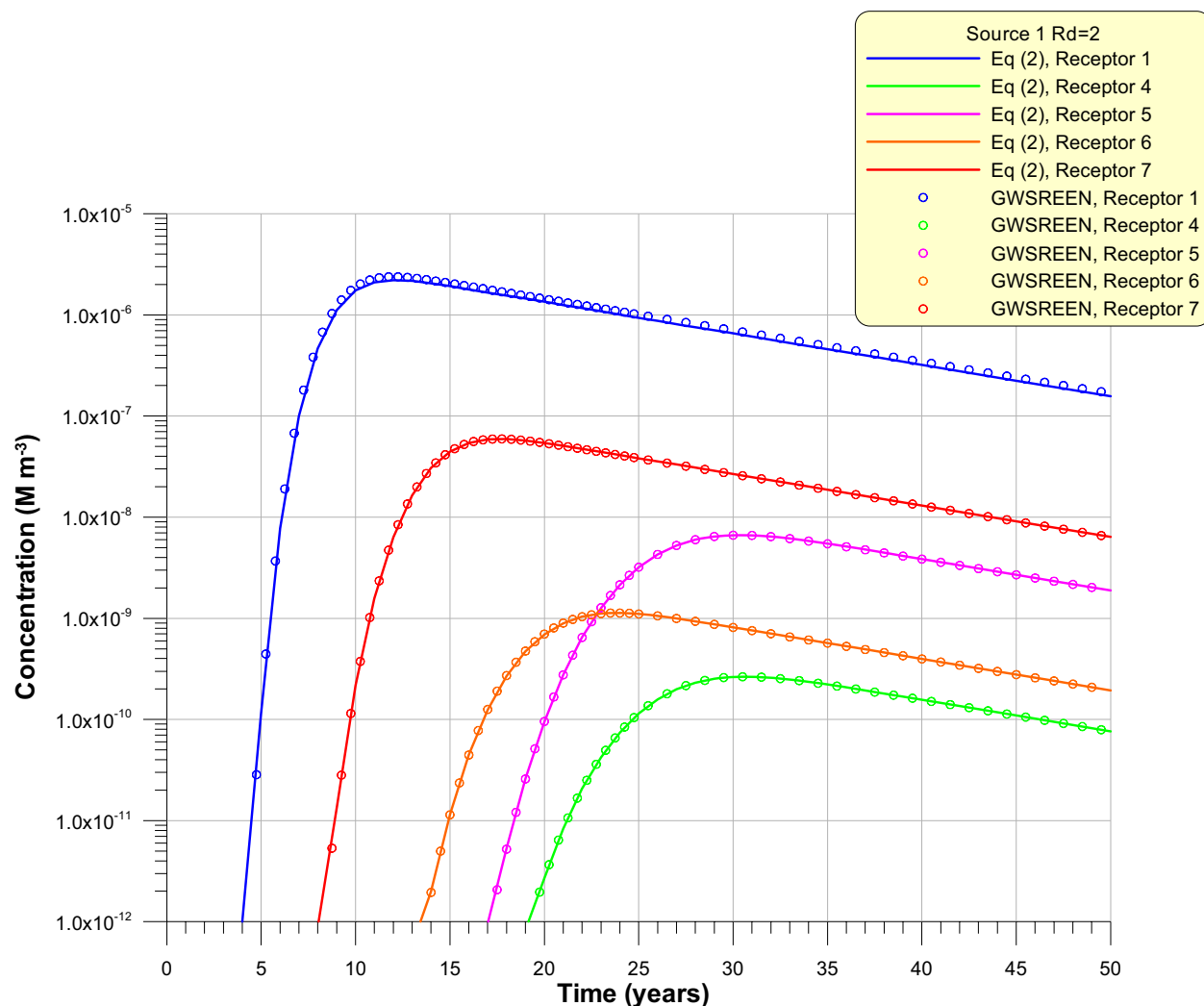


Figure 5. Contaminant concentration as a function of time for Source 1 and a contaminant having a retardation coefficient of 2. Compare with the graph for Source 1 in Figure 4.

Two individual sources and six receptor locations were considered for this application (Figure 6). The contaminant simulated was tritium (H-3, half-life = 12.3 years). One source was placed at the Idaho Nuclear Technology and Engineering Center (INTEC) and the other at the Radioactive Waste Management Complex (RWMC). The INTEC source has been designated WAG 3 and the RWMC source has been designated WAG 7. Historical releases of tritium at INTEC have occurred since 1952 and significant quantities of tritium have been disposed of at the RWMC. However, the tritium source-loading rates for WAG 3 and WAG 7 that are illustrated in Figure 7 are only for demonstration of the model and do not necessarily represent the current or best understanding of tritium releases from Idaho National Laboratory facilities.

Response functions were developed for each of the six receptors for the WAG 3 source (Figure 8) and the WAG 7 source (Figure 9). Note that three of the receptors lie upgradient from WAG 7; therefore, the response functions for these receptors are zero for all times. Response functions were developed from the data in Table 1. The concentration as a function of time output from MT3D was converted to a unit response function by dividing the groundwater concentration at a receptor by the initial mass placed in the aquifer at the start of the simulation.

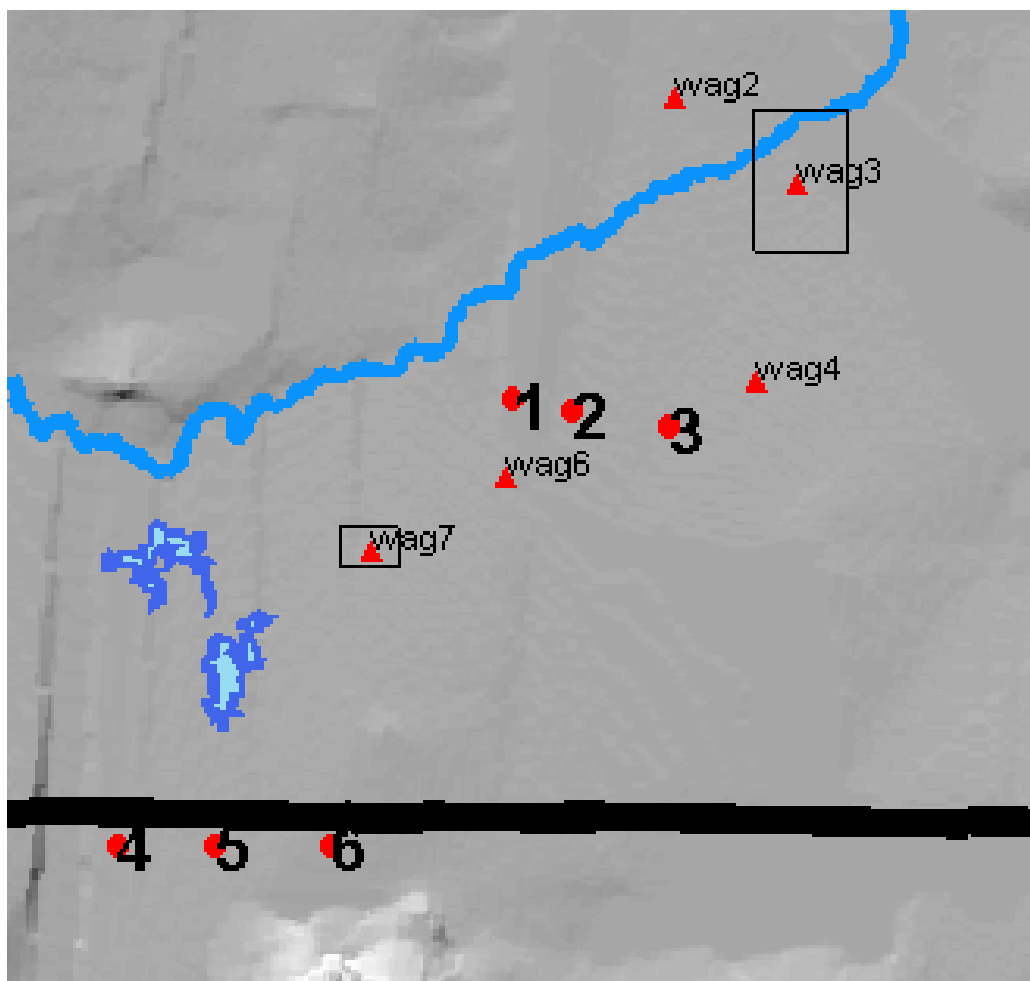


Figure 6. Map of the southern portion of the U.S. Department of Energy Idaho Site showing the location of the Radioactive Waste Management Complex (Waste Area Group 7) and the Idaho Nuclear Technology and Engineering Complex (Waste Area Group 3) and the six receptor locations used in the response surface modeling application.

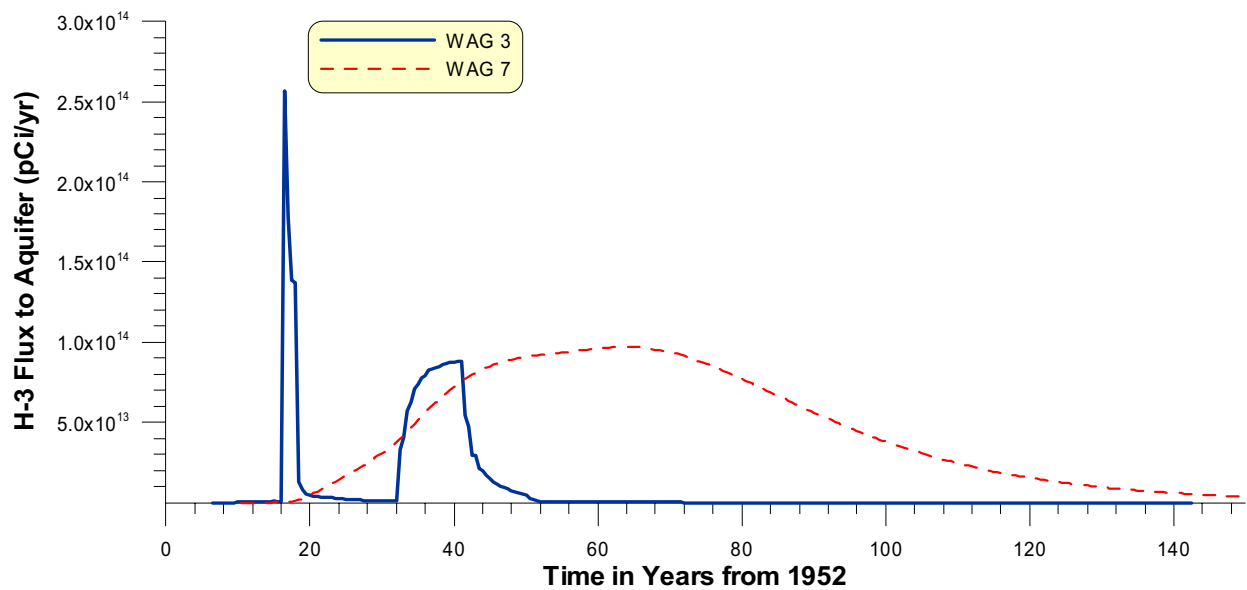


Figure 7. Tritium source-loading rates from Waste Area Group 3 (Idaho Nuclear Technology and Engineering Complex facility) and Waste Area Group 7 (Radioactive Waste Management Complex).

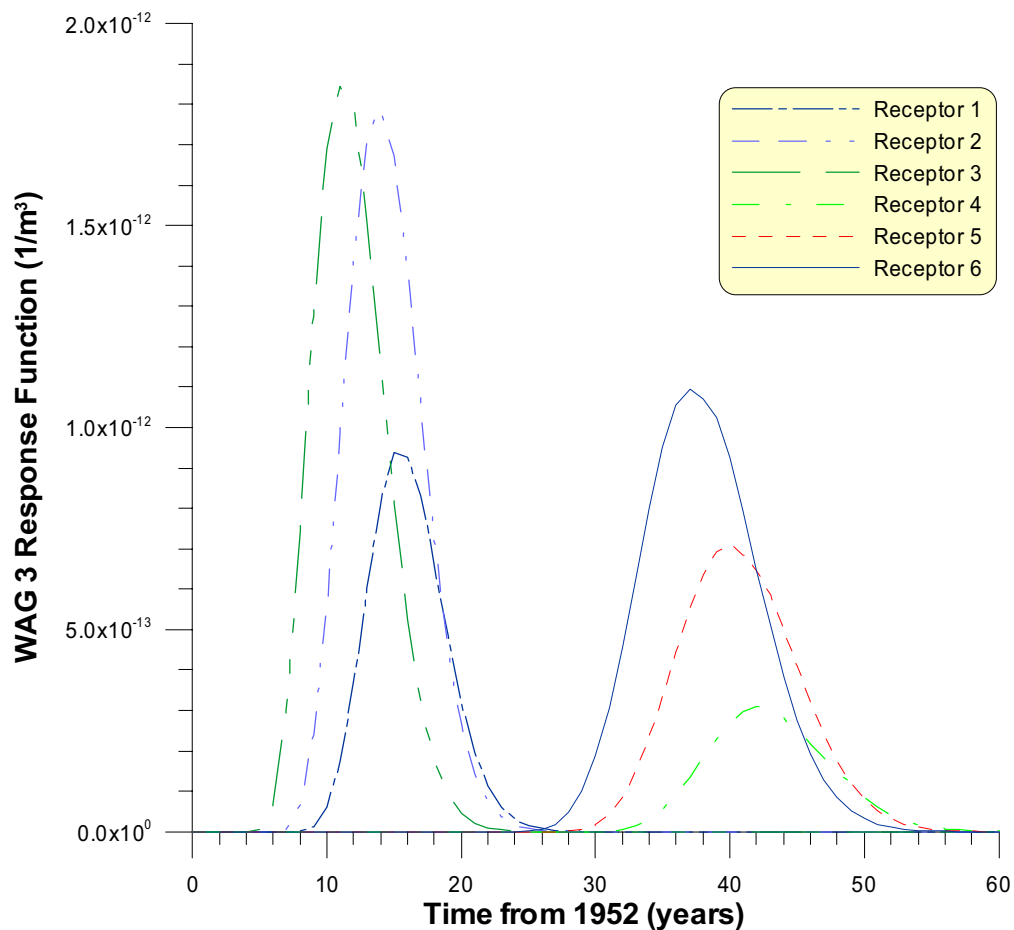


Figure 8. Response functions for Waste Area Group 3 sources at the six receptor locations calculated with the MODFLOW/MT3D model.

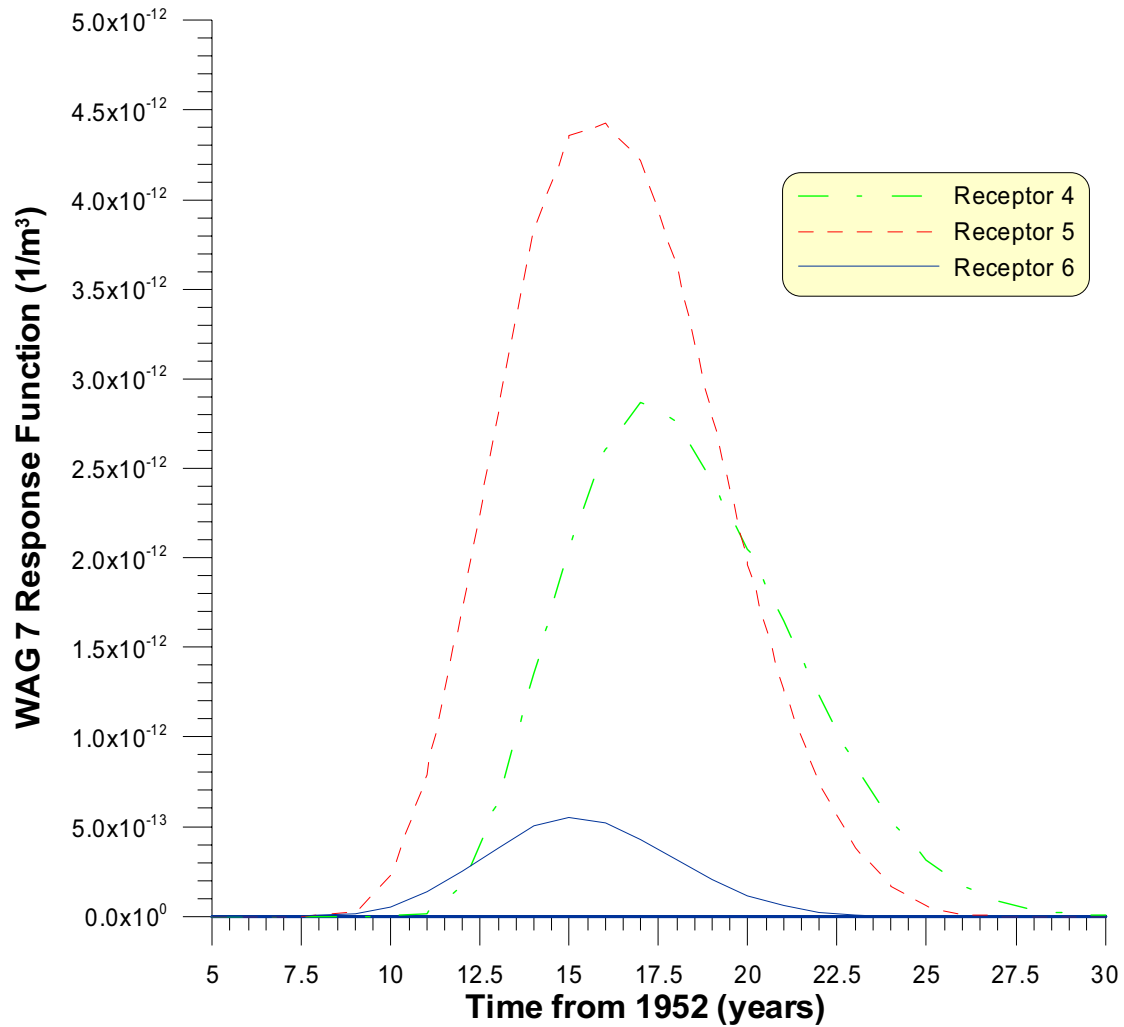


Figure 9. Response functions for the Waste Area Group 7 sources at the six receptor locations calculated with the MODFLOW/MT3D model. The response functions for Receptors 1–3 were zero for all times.

Table 1. Data used to develop the response functions for Waste Area Groups 3 and 10.

Parameter	WAG 3 Value	WAG 7 Value
East-west length (m)	2,000	1,219
North-south length (m)	3,000	915
Aquifer depth (m)	285	142
Porosity	0.15	0.15
Initial concentration (mass/L)	10,000	10,000
Volume of water in source (L)	2.565×10^{11}	2.3758×10^{10}
Initial mass (mass)	2.566×10^{15}	2.37577×10^{14}
WAG = waste area group		

The results of the response function simulations for tritium are illustrated in Figures 10–12. For comparison, tritium transport also was performed using MODFLOW/MT3D, and these results are plotted alongside the response surface model results. Differences between the *maximum* tritium concentrations estimated with the response surface model and those estimated with MODFLOW were no greater than 6% and typically were less than 3%.

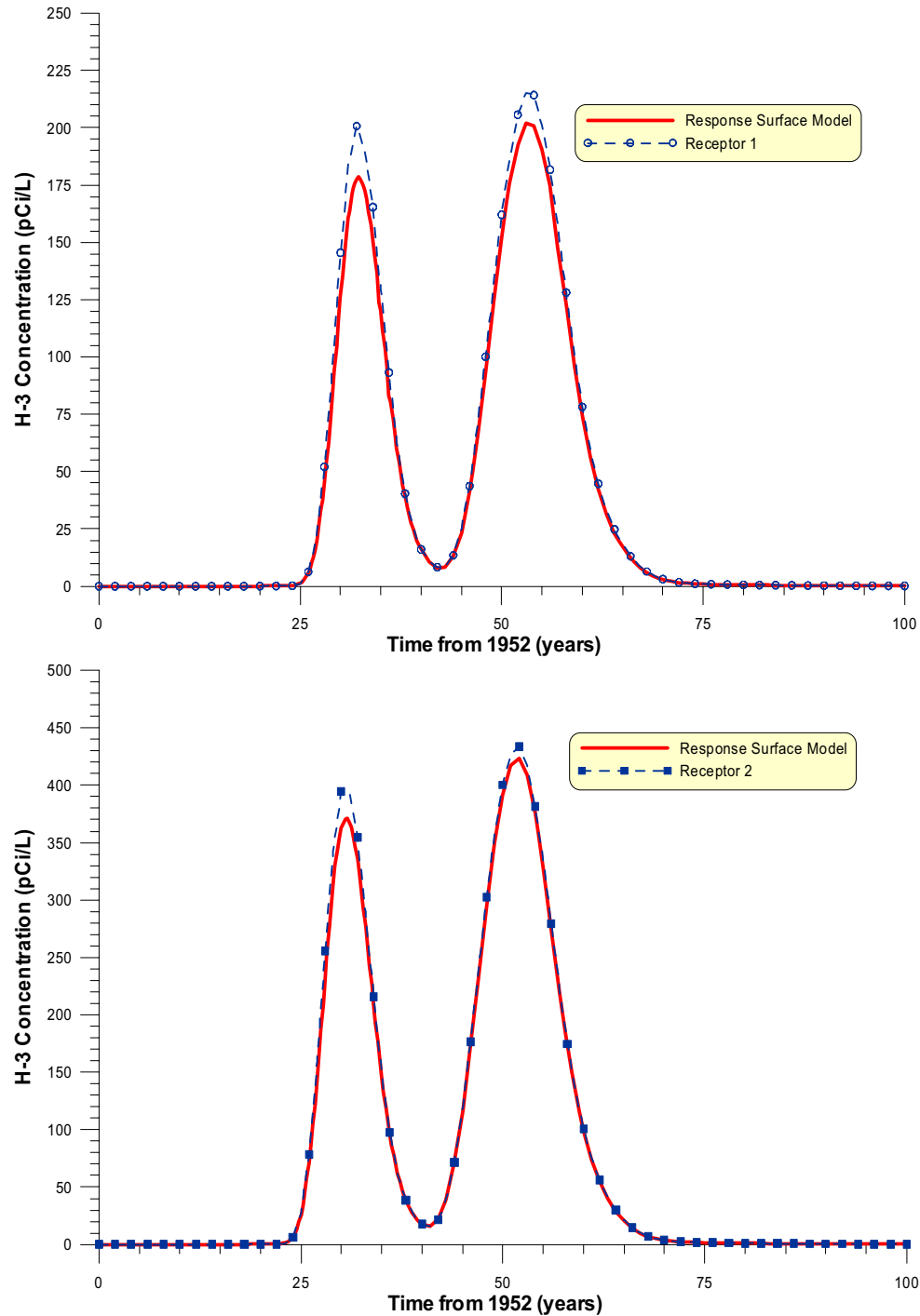


Figure 10. Comparison of MODFLOW/MT3D and response surface model for model-predicted tritium concentrations in the Snake River Plain Aquifer at Receptor Locations 1 and 2.

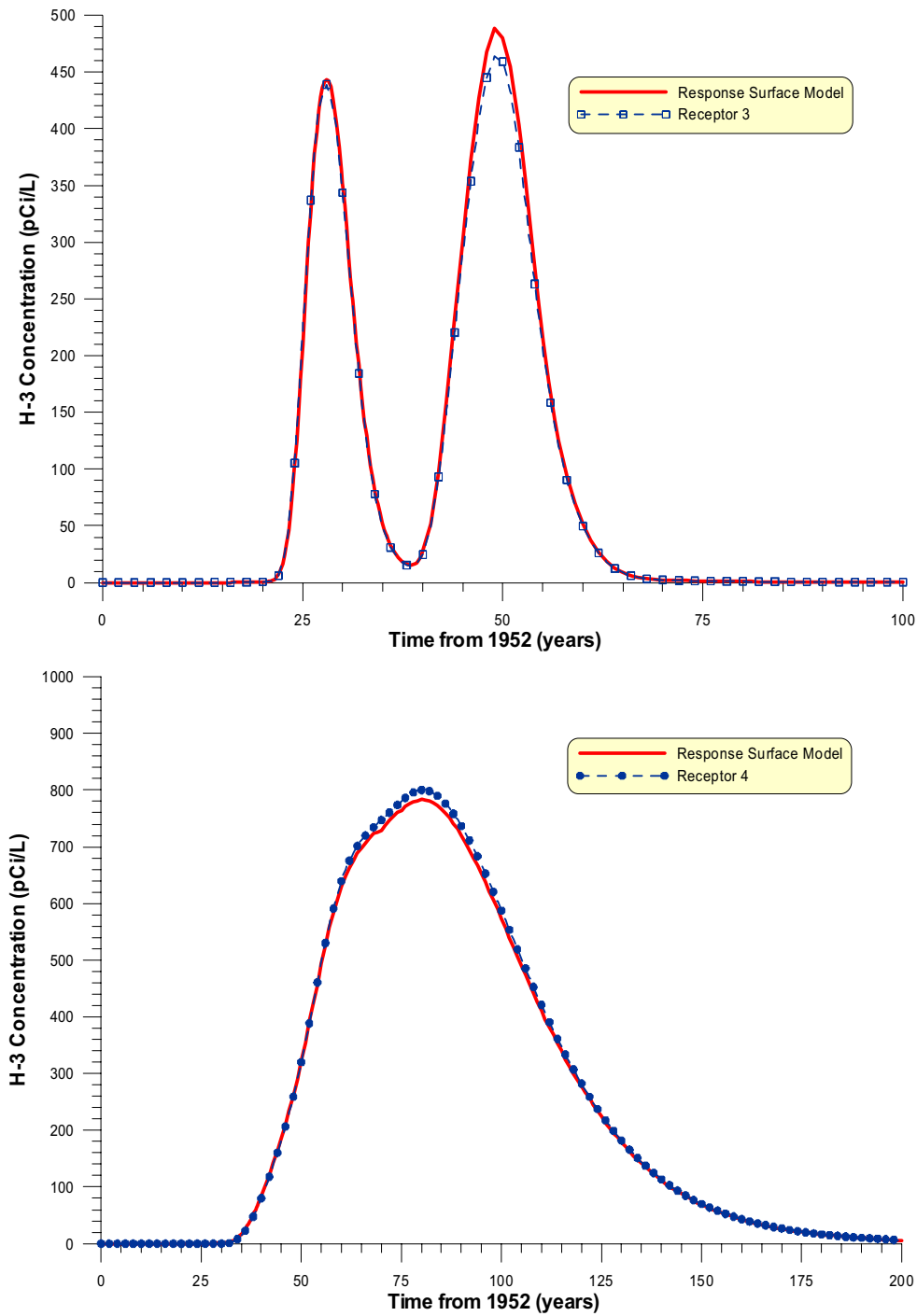


Figure 11. Comparison of MODFLOW/MT3D and response surface model for model-predicted tritium concentrations in the Snake River Plain Aquifer at Receptor Locations 3 and 4.

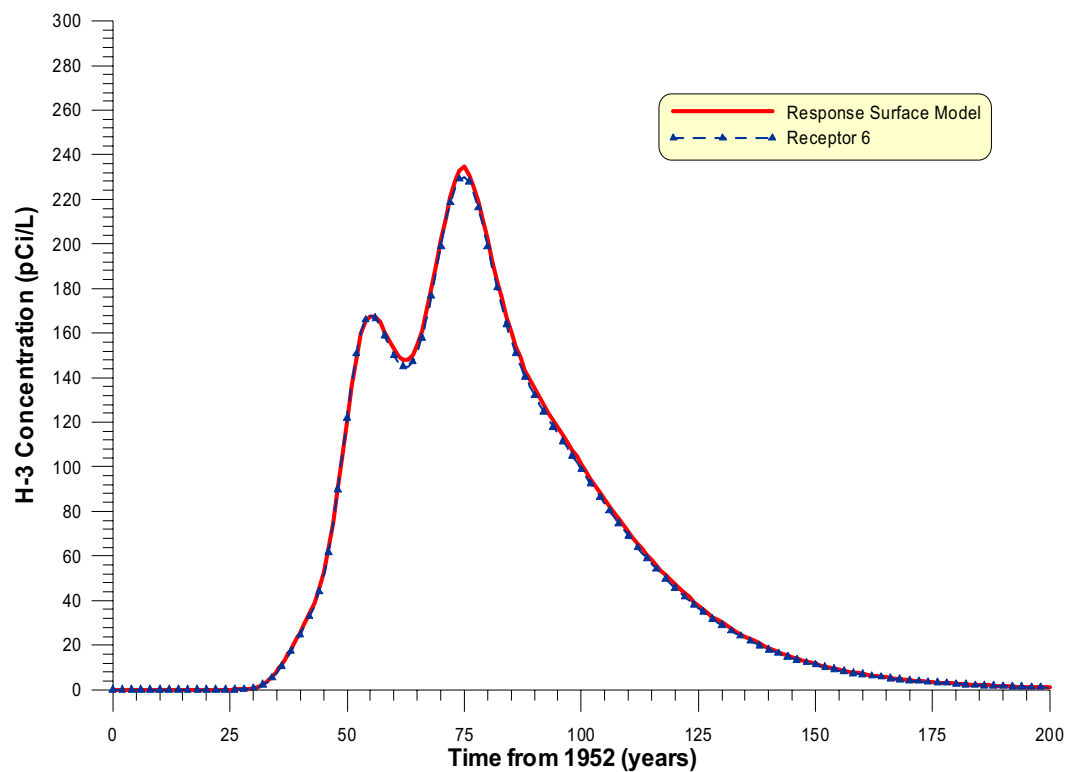
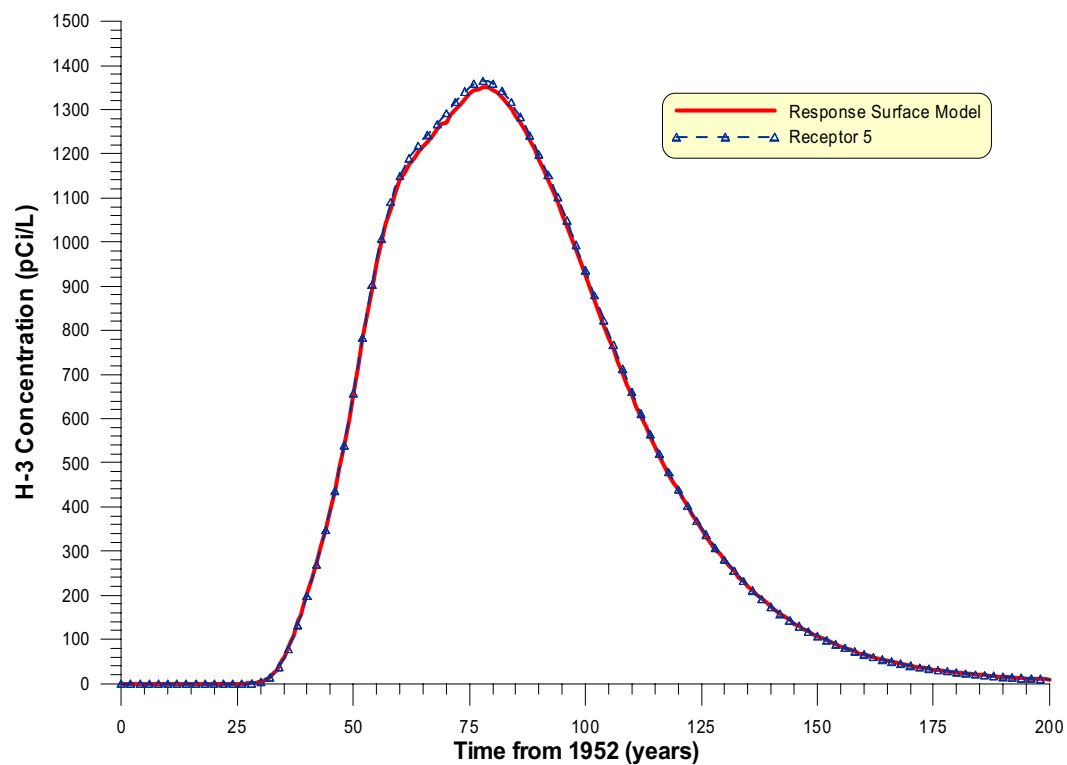


Figure 12. Comparison of MODFLOW/MT3D and response surface model for model-predicted tritium concentrations in the Snake River Plain Aquifer at Receptor Locations 5 and 6.

6. SUMMARY

In summary, the response function method discussed here is a viable method to incorporate a relatively complex groundwater flow and transport model into an assessment framework that considers arbitrary source-loading rates for numerous sources and contaminants.

7. REFERENCES

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- Rood, A. S., 1999, *GWSCREEN: A Semi-Analytical Model for Assessment of the Groundwater Pathway from Surface or Buried Contamination, Theory and User's Manual Version 2.5*, INEEL/EXT-98-00750, Rev. 1, Idaho National Engineering and Environmental Laboratory, February 1999.